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The research accomplishments during the 3 years of the project covered three areas: Emulsion Science and Technology Cluster; Flavor Science Technology; and Process Control and Simulation. The project leaders, students involved and the results are appended.

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Executive Summary

EMULSION SCIENCE + Technology Cluster

The overall goal of the emulsions science and technology cluster is to establish a template for the design of heat, shear, and oxidation stable emulsions. The specific goals are:

- to shed light on the mechanism by which proteins and antioxidants participate in stabilizing food emulsions relative to flavor and separation,
- to develop a scale of antioxidant efficiency for food emulsions and to evaluate the efficacy of natural antioxidants, and
- to develop and experimentally evaluate a computer based method for predicting the potential efficacy of proteins to function as emulsifiers.

A two pronged approach was adopted for the development of the emulsions science and technology cluster. The design of a computer based method for predicting the efficacy of protein in emulsion stability and further definition of the arenediazonium ion probe for identification of the components in the interfacial region of an emulsion would be progressed simultaneously. These method development tasks will provide the basis for increased understanding of the role of proteins and antioxidants in emulsion stability.

A broad and critical review the scientific literature pertaining to food emulsions was undertaken so as to generate a biophysical and biochemical view of published results which could be a useful guide to the future directions of the research effort. Examination of about fifty publications demonstrated clusters of investigation in competitive effects of surfactants and proteins in emulsions, interactions between proteins and surfactants in aqueous solutions, protein adhesion to oil droplet surfaces in emulsion interfaces, and covalent chemical reactions in emulsions. Some key conclusions were that protein emulsions are more stable than surfactant emulsions, isoelectric points of proteins change as a function of conformational changes, unfolded proteins show increased dependence upon salt and pH, the scientific understanding of emulsion surfactants is greatest for anionic surfactants, less for cationic surfactants, and least for non-ionic surfactants, food systems are most often based upon non-ionic surfactants, surfactants force proteins into the aqueous phase, oxidation of thiols is promoted by cationic surfactants, sorbic acid, and heavy metals but is inhibited by low pH , and chemical reaction rates in bulk fluids differ from those in emulsions. The development of the literature review is continuing.

The development of the computer based model for efficacy of proteins in emulsion stability was advanced through the development of a molecular modelling laboratory with thirteen interconnected work stations. The sequences of several proteins were downloaded and the software for determining Chou-Fasman helix and strand potentials and Garnier-Robeson helix potentials was obtained.

Research on the arenediazonium ion probe demonstrated that it is able to quantitatively trap water, alcohols, halide ions, carboxylate ions, aromatics, proteins, and tocopherols.

Therefore the probe can search the interfacial region of emulsions for numerous components of food emulsions, including flavors, salt, vinegar, antioxidants, and emulsifiers. Some interesting conclusions of the research were that thermodynamic stability of emulsions is increased as the hydration of the interface is increased, that the rate of protonation (reduction of the oxidized arene) by alpha tocopherol is twice as fast as the rate of protonation by an oxidized arene in an emulsion, and that the probe traps amide nitrogen and amide carboxylate in a model protein indicating the potential for describing protein topology in the interface.

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FLAVOR SCIENCE TECHNOLOGY

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Executive Summary

FLAVOR SCIENCE TECHNOLOGY

An apparatus for measurement of dynamic flavor release from food in a simulated mouth model system was constructed. It was designed to perform dynamic measurements of flavor release taken in the short time frames typical of eating foods. It has ultra high sensitivity modes of detection for trace levels of flavors expected to be released. Preliminary data obtained from a 60 second measurement made on a 5g sample of pound cake using the mouth model system apparatus are successfully presented.

Research on understanding the kinds of diffusion regimes encountered during typical storage conditions and developing predictive methodology for diffusion of flavors with different molecular weights and functional groups in food matrices was attempted. Both experimented method using IGC and theoretical estimation of diffusion coefficients are studied.

Mechanisms for the formation of important bakery flavor components, 2-acetyl-N-heterocycles are studied. The acetylpyrazine generation in nine model reactions containing amino acid (serine, threonine, or glutamine) and monosaccharide (glucose, fructose, or ribose). It was found that acetylpyrazine, a potent roasted, popcorn-like aroma was proposed only in glucose- and fructose- containing systems and not in ribose- containing systems.

Thermal degradation products of methional under different temperatures were identified. Research plan for the study of the chemical kinetics that affect the storage stability of methional in starch base food systems is designed.

Methional is an important characteristic flavor in potato products. The precursor for methional is free methionine in potato. Attempt to increase the free methionine level in potato through biotechnology is made. Twelve independent transgenic potato lines were generated. Eight of these lines were analyzed and four different transgenic lines had higher levels of CGS (cystathionine γ-synthase) than the wild type control plants

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Executive Summary

The Process Control and Simulation cluster is a part of CAFT's new Cooperative Research and Development program, which was reorganized in the Fall of 1997.

The objective of the Process Control and Simulation cluster is to develop and demonstrate the control and optimization tools for selected processes such as extrusion and baking. Over the last several years CAFT has developed substantial knowledge base and know-how on extrusion cooking, material science and advanced sensing technology. Therefore, the extrusion process was chosen as the process for which an intelligent process control strategy will be developed to demonstrate delivery of high quality processed food with optimum utilization of the resources.

An effort has begun to model and quantify the judgments of a master extruder operator and the resultant actions taken. The overall goal is to sense how the operator reacts, make similar judgments and take similar actions using a process controller that can learn and incorporate the knowledge base of the operator. New types of neural net-based controllers show strong promise of meeting such a goal of intelligent control.

The neural net program will make use of the knowledge coming from the continued numerical simulation efforts through guidance for net model selection and through performance improvement with a broader input/output range without an extensive number of experiments. In this regard, the validation of the mathematical model and computer code has been achieved through good agreement between experimental and numerical results on velocity distributions in screw channels. The coupling between chemical reactions, flow and heat transfer have been investigated.

A wide range of operating conditions have been simulated to determine the feasible domain for the operation of twin-screw extruders for different materials. This information will be very useful in developing the control scheme without having to run extensive experimental tests to obtain input/output variations for the neural net model. Work has also been initiated on the transient processes since these results are needed as inputs for the control system

Flow characteristic curves for a single hole die used in conjunction with a ZSK-30 extruder were obtained. The materials tested were corn syrup and Amioca corn starch, the properties and rheology of which are well defined. Results compared well with theoretical predictions, for isothermal conditions. The results from the die simulation will be combined with the results from the numerical simulation for screw to generate operating points for the extruder.

Online moisture determination of ingredient flour moisture is believed to be a significant factor in avoiding out of spec product excursions. Adaptation of the CAFT invented Thermomoisture probe is being addressed on two fronts. A study of potential sampling systems led to selection of a vibrating flour compactor that will be designed and tested. Improvements in instrumentation electro-mechanical component design have shown increased reliability in sensor measurement needed for a robust field useable system.

To provide a product quality input to the neural net-based control program, we have selected the pyrazine sensor. In the last six months the research on Pyrazine flavors has progressed such that a signal from peanut butter can be obtained within 10 minutes at 60°C. This a substantial improvement over the past results where 60-90 minutes were required to observe similar signals. The new polymer electrodes are expected to be independent of food matrix. We expect to further reduce the time of measuring Pyrazine flavors to 1-2 minutes through sensing material optimization and sampling system improvements.